Atomic and Molecular Physics

Prof. Amal Kumar Das
Department of Physics
Indian Institute of Technology, Kharagpur

Lecture 43
Rotation of a molecule (Contd.)

So, we are discussing about the rotation of a molecule, means rotational spectroscopy. So thaw can tell about the microwave spectra. So, what we should do, as we have seen that there are different kind of molecules. One is linear molecule and one is linear molecule. In respect of rotation, this division is very important. So one is linear molecule, where Iy equal to Iz and Ix equal to 0 and then, your other polyatomic molecules, where some of them are symmetrically top molecule or spherically top molecule or asymmetric top molecules. So that I have defined, I have differentiated; with respect to moment of inertia principle moment of inertia.

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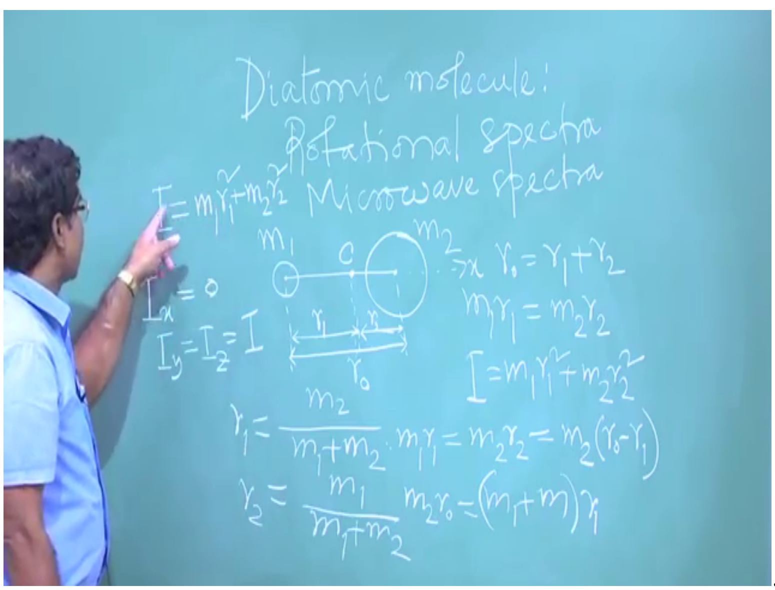

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So basically, we will study here mainly, because this is the simplest one, simpler one this diatomic molecule- rotation of a diatomic molecule, diatomic molecule, ok. So it is diatomic molecule. So, which will give you rotational spectra and of course, it is in its spectra, it is in microwave. So, it is also called microwave spectra, which is common for all molecules, all rotational molecules. So, microwave spectra. So, that is what we would like to see: what is the origin of these spectral lines, of these spectra, of this radiation. So, for that, we have to we have to study this. We have to study the rotation of these molecules and simplest molecules, as I have chosen, that is the diatomic molecule, because it has only one moment of inertia. So, you take a problem now. So, we have to use quantum mechanics, we have to solve, we have to find out the energy of the rotational diatomic molecule or energy of or rotational energy of diatomic molecule.

So, we have to consider the rotation of the body systems, two mass systems right? In general just consider two mass. Consider these two mass having different mass. So, one is m 1 and another is m 2 right? And their separation is, separation is say, is separation is at zero. Say r 0. This is, basically the bond length and now, for these two body systems, let us guess, let us take, let us reduce the two as one body system. So, that is, you know how to do that? So, one has to find out the reduced mass. So then, it would be converted to the one body system. So, for that one has to consider center of gravity. So from center of gravity the distance. So, this distance say r 2 and this distance say r 1 right? So now, you know this. Just put r 0 equal to r 1 plus r 2 and then, m 1, r 1 equal to m 2, r 2. So, that is the r 1 r 2 distance of the mass from the center of gravity. Now, you have this 2 r 0 equal to r 1 plus r 2 and m 1 r 1 equal to m 2 r 2, right?

So, from these two, yes one can and also, I know that this moment of inertia, in this case linear. So this is the x axis. So, basically Ix equal to 0 and Iy equal to Iz, equal to I have written I. So, I equal to is, basically moment of inertia which is this, the Iy axis and this other one, is perpendicular to Iz axis. So I, it can be either Y direction or with respect to Y1, direction or Z direction, so both are, I think the same. So, I will be moment of inertia with respect to this axis, passing through the center of gravity. So, distance is r 1 –R 2. So, moment of inertia will be basically m 1 r 1 square plus m 2 r 2 square, right? So, these are the things. So, here I can write, I equal to m 1 r 1 square plus m 2 r 2 square right.

So, from these three relations, you can, I will not just derive, but it is, you can just easily; I think I can show you. Let me do it. m 1 r 1 equal to m 2 r 2. So r 2, I can replace r 0 minus r 1. So m 2, r 0 minus r 1. So, from here what you will get? So m 1, r 1 here, m 2, r 2 minus m 2, r 2. So m 2 r 2 if I take this side, so then, I will get m 2, I will get m 2 r 0 equal to m 1 plus m 2 into r 1 equal to by r 1. So here r 1. What I am getting? r 1 equal to m 2 by m 1 plus m 2. Similarly, just from here itself, you replace r 1 by r 0 minus r 2. So you can show that, it will be m 1 by m 1 plus m 2, right? So, I equal to m 1. So now, r 1 square, if you take this. So, m 1 r 1 square means m 2 square.

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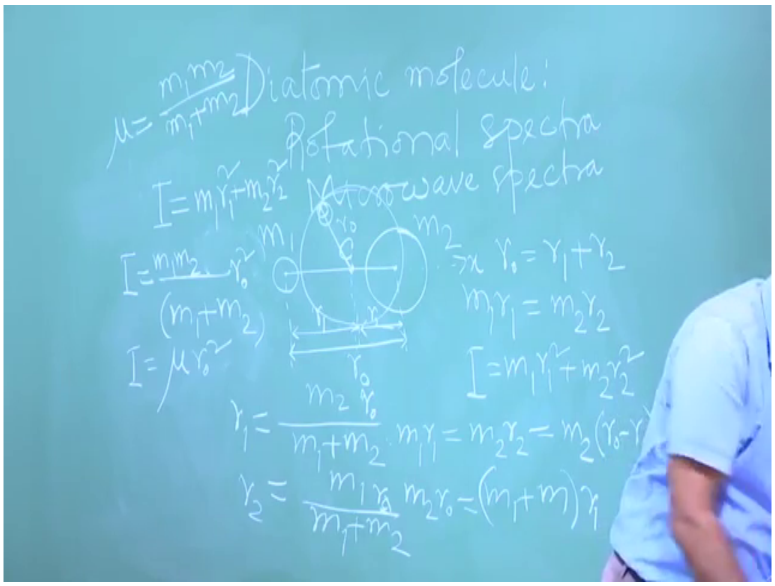

So I think, I will here itself, I can write. So, your I will be, so here, I am getting m 1 m 2 square and divide by m 1 plus m 2 square plus m 2, I am getting r 2 m 1 square divided by m 1 plus m 2 square. So, m 1 plus m 2 square in both cases and m 1 m 2, I can take common, then, there will be m 1 plus m 2. So basically, this square will go. So, it is m 1 m 2 plus m 2 and for all cases. So I 0, I have not written.

So, there will be r 0 in both cases. So, this square of this means r 0 square will come, r 0 square will come here. So here, these you can write I equal to m u 0 square. So, m u is the reduced, so, m u equal to, so m u equal to basically; you have m 1 m 2 divide by m 1 plus m 2. Now, as if we have one body problem. So, we have mass m u. Now, it is moment of inertia. This mass is rotating with respect to yes, so, as if I take this center. So, I have another mass. So, mass m u. So, this mass with respect to it is rotating, it is rotating and this length is r 0. So now, it is reduced to one body problem. So basically, you have now, problem like these. So, I basically have, I have reduced these two body problem to one body problem.

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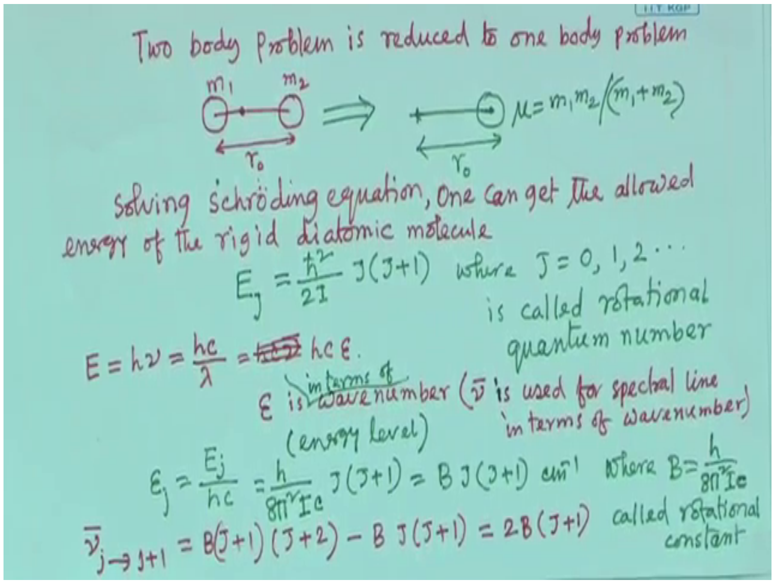

So, two body problem is now reduced to one body problem, right? So now, this is our system. Now this, see this, it is just like hydrogen, in how to solve this kind of problem that we are seen, as it is hydrogen like atom. So, they are basically nuclear mass and the electron mass and we have taken their reduced mass. So now, this is the same kind of problem, only difference is that in case of hydrogen like atom, there was a central potential. So, v r equal to minus J d square by r and now in this case, this v r is basically 0.

So, there is no potential energy, only kinetic energy rotational kinetic energy. So, one can one can use (Refer Time: 13:33) equation and solve it in same way and now imagine there. So, r 0 in this case, it is how to consider this one is, so, I think this, I have to; here I have not told you. So, one thing I have to tell that, this now when it is, molecule is rotating, now this, there are two model you know, one is called rigid rotator; one is called rigid rotator. So, this basically there are two model for calculation of this or solving the (Refer Time: 14:44) equation.

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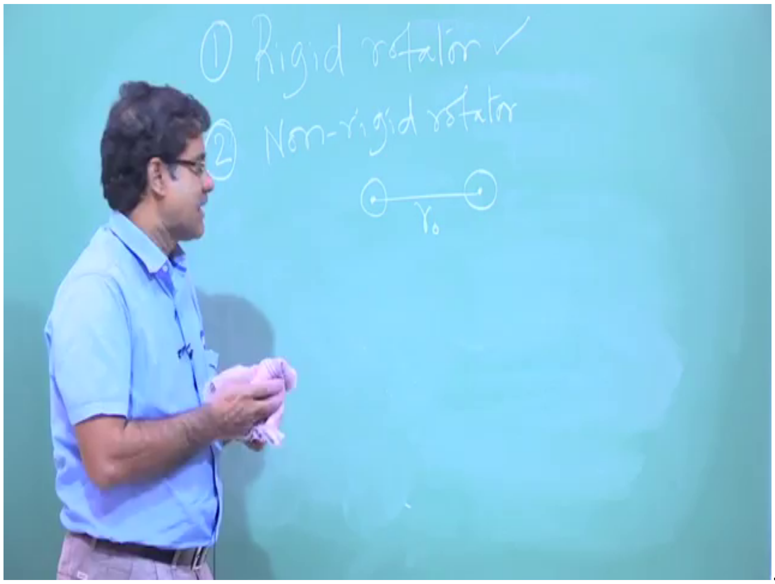

One is called rigid rotator and another model is called non rigid rotator. Non rigid rotator what is this? So rigid rotator! So, you have molecule, having the bond length is r 0. Now, if this distance remains same all the time, it is these two atoms are tightly bound with each other. So there, this bond length does not change during rotation. So, then it is called rigid rotator, but there are some molecules or most of the molecules, basically it is not, that rigid. So, during rotation, its bond length also changes.

So then, it is called non rigid rotator. So this non rigid rotator is basically, it is the realistic model. Non rigid rotator is basically not realistic, but for the simpler calculation, let us first consider this rigid rotator and then, later on we will see what effect due to the change of bonding, or when it will be the non rigid rotator. So, what will be the additional effect, we will see, so that we will discuss later on. So, now let us take it is a rigid rotator. So, when it is rigid rotator. So, basically r 0, this length, it will not change right? In case of hydrogen atom, so r was variable and theta phi.

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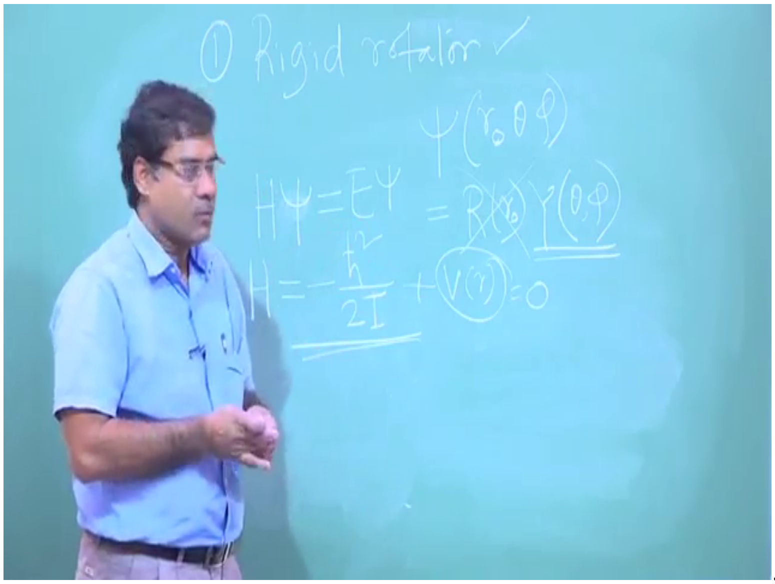

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So phi, so, this function phi is basically a function of r theta pi. So, in this case, in case of rigid rotator, this r is basically rigid, r is constant. So this, what was the phi r theta phi? So, it was basically r R function also in the hydrogen like atom, we have seen theta phi right? It is a spherical harmonics, theta and phi dependent and this is, one part radial dependent. So, in this case this r to r 0, it is constant. So, basically there will not be change of this one. So only this is the right way to function, this can also be a function, but it is the active one, it is this, which will participate in the, yeah! So, this part is active. So basically, this is nothing, but that, what is the solution for this kind of wave function.

So, they are here in this case. This H is Hamiltonian H. So, always showing an equation: H psi equal to E phi. So, one has to find out proper phi Eigen function and then, for that, for your system you have to write your this Hamiltonian. So, our Hamiltonian will be only kinetic energy h plus square by 2. Now here, you see, I will not write 2 M, right because I have already told, in case of rotation mass is not important; important is basically I. So, here I will write I h square by 2 I in place, where ever mass will be there, I will be replaced by 2 I. So h square by 2 I. So, that will be our Hamiltonian plus your V is termed. So, that is basically 0.

So, if you apply these Hamiltonian on these. So, these basically it will. So, this one can show this is kinetic energy, it is basically kinetic energy rotational, it is the angular. So, this energy comes due to the angular motion, its rotation motion its nothing but the angular motion. So, one can show that, this energy is kinetic energy, basically it is due to the angular momentum. It comes from the angular momentum, not linear momentum. So what about the things? So, if you solve this, solving this equation I will not go into details. So, you solve this equation and you will get basically this type of regent, here I am showing you. So, solving Schrödinger equation, one can get the allowed energy of the rigid diatomic molecule. So, E J equal to h square by 2 I J J plus 1.

So, it is similar to l l plus 1 right? So, angular momentum, so, in this case energy expression you will get for this rigid rotator, solving the Schrödinger equation, this energy expression will get this. So, where J is basically, it is called the rotational quantum number. So, it is equivalent to l basically. So, if this is the energy. So, now, in terms of wave number, I want to write this energy. So, in terms of wave number, so, E is equal to nu is C by lambda. So hc1 by lambda, I have retained here, energy basically wave number in place of nu bar. I have written small e, in different different letter, different form of hc E, we will tell it is e, but it is, you can say this, there is, a just both are e, but we have written different, what is called this different font basically.

So, this E is basically the wave number, e is in terms of wave number of energy level. Energy level is expressed in place of just electron bolt or joule. We have expressed in terms of centimeter inverse energy level. So, that is expressed by e and new I, have energy new bar is used. So, nu bar I have avoided because to avoid the confusion. So, nu bar will use the energy of the spectral line. So, basically, two energy level whatever the transition. So, due to that transition, I will get the spectra or radiation; that radiation will have the frequency or energy. So, that will express in terms of wave number and there will you use nu bar.

So that is basically energy of the spectral line. Your nu bar is will be used to express the energy of the spectral lines and here e, this e is used to express the energy level in wave number. So, if e equal to hc E. So, this I can write EJ equal to EJ by hc equal to h square means, h square plus 4 pi square, 2 is there eight, pi square IC divide by hc is h square and this divide by 8. So, it is h by 8 pi square ICJJ plus 1. So this, the energy level comes in centimeter inverse. So this B, so, we have written here B. So, B is nothing, but a constant. You see here, all are constant for a particular molecule. So, this B is equal to h by 8 pi square IC. So, it can count I, ok?

Moment of inertia so now, these spectral lines, how many will get due to the transition between two energy levels. So, what will be the energy of the spectral lines, so, that we are expressed in terms of nu bar equal to nu bar. So, this nu bar due to transition from J to J plus 1 or J plus 1 to J between this, successive to energy levels. So, that is basically, so this energy levels, that energy in terms of wave number. So BJJ plus 1. So, I can write JI can replace by J plus 1. So, it will be BJ plus 1J plus 2 minus J equal to J. So BJJ plus 1. So, it is giving 2BJ plus 1. So, this is the energy of the spectral lines in centimeter inverse, or in terms of wave number, ok. And this B is called basically rotational constant. So here, nicely to we got the, yes this energy of the or wave number of the spectral lines of rotational spectra.

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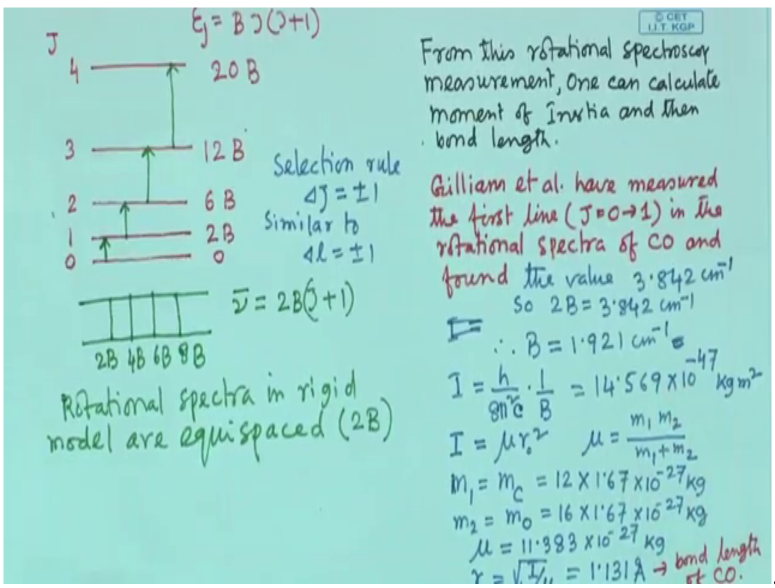

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So, if I plot it. So, EJ equal to BJJ plus 1. Now, just if I draw the energy levels in centimeter of inverse, of course. So, J equal to 0. So, this is the 0 energy, J equal to 1. So, it will be JJ plus 1, it will be 2, so 2B. So, this 2B then, J equal to 6B, 12B, 20B. So, that is the energy level in terms of centimeter, inverse in terms of B we have shown. Now, when there will be congestions, that selection will be similar to that angular momentum selection rule ll equal to plus minus 1. So, here same selection rule is valid DEl J equal to plus minus 1. So if delta J equal to plus minus 1.

So, so from 0 levels J equal to 0 to J equal to 1, this transition is possible or 0 to 0, that is also possible. So, 0 to 2 0 to 3 0 to 4, it is not allowed. So, this transition, it will give one spectral line.

So next is 1 to 2, 2 to 3, 3 to 4. So, we will get the corresponding spectral lines and energy of the spectral lines are 2B, here 4B, here 6B, here 8B; that means here, I will get spectral lines and spectral lines are equally spaced; equispaced and this difference between two spectral lines, this is 2B. So, from rigid rotator model, we will get the spectra, we will get the spectra of diatomic molecule, linear molecule and it will give equispaced spectral lines and difference between the successive spectral lines, that is 2B. So, next class I will continue this discussion on this issue,

Thank you.